ISSN 1063-7761, Journal of Experimental and Theoretical Physics, 2008, Vol. 106, No. 4, pp. 752–764. © Pleiades Publishing, Inc., 2008.
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NUCLEI, PARTICLES, FIELDS, GRAVITATION, AND ASTROPHYSICS

Dynamic Spin Susceptibility of Hole-Doped High-Temperature Superconductors in a Singlet-Correlated Conduction Band Model

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Received July 2, 2007

Abstract—We have derived an expression for the dynamical spin susceptibility of a hole-doped high-temperature superconductor taking into account a strong correlation between the magnetization of spins of the localized and itinerant electrons. This formula has been used to calculate the imaginary part of the susceptibility as a function of the frequency and wave vector. The results are compared to experimental data on the inelastic neutron scattering in compounds of the $YBa_2Cu_3O_{6+y}$ type. A peak in the scattering intensity observed at an energy of about 40 meV in the region of wave vectors $Q = (\pi, \pi)$ and an arc-shaped dispersion relief are interpreted as manifestations of the collective spin excitations in the system, the energy of which falls within a superconducting gap (spin exciton). The U-shaped divergent relief observed in the neutron scattering intensity is assigned to collective short-rage-order spin oscillations.

PACS numbers: 71.27.+a, 74.72.-h

DOI: 10.1134/S1063776108040146

1. INTRODUCTION

At the present stage of the theory, there are two main approaches to the treatment of magnetic susceptibility of high-temperature superconductors (HTSCs). The first approach is based on the well-developed theory of metals and takes into account strong correlations inherent in HTSCs within the framework of the random phase approximation (RPA). In application to descriptions of inelastic neutron scattering, this approach succeeded in explaining the nature of the resonance peak observed for the superconducting phase in the region of wave vectors $Q = (\pi, \pi)$ at a neutron energy of about 40 meV [1]. This peak appears as a result of vanishing of the real part of the denominator of susceptibility, whereby the root frequencies fall in the transparency region due to a *d*-wave superconducting gap. In compounds of the $YBa_2Cu_3O_{6+y}$ type, the transparency region for wave vectors $Q = (\pi, \pi)$ amounts to 60–70 meV [2]. The main parameter in calculations using the RPA scheme is the carrier exchange parameter U, which is usually on the order of 0.2–0.3 eV [3, 4]; however, the microscopic nature of such values of U still remains unclear.

Another popular microscopic approach to description of the electron structure of the conduction band in HTSCs is based on a model employing composite (Hubbard type) operators of generation and annihilation of current carriers [5, 6]. A considerable advantage of this model is that it describes the insulator–metal transition taking place in these compounds. Based on the photoemission and NMR data, it is believed that the current carriers in hole-doped HTSCs are distributed predominantly over oxygen sites. A strong exchange interaction between itinerant holes on the oxygen sites and localized holes on the copper sites splits the oxygen band into two subbands. The lower subband exhibits clearly manifested singlet correlations between holes on the copper and oxygen sites (singlet-correlated band model) [7–9]. As for the Hubbard operator technique, this band can be considered analogous to the upper Hubbard subband. The parameter of exchange interaction between copper spins is expected to be approximately equal to an analogous quantity in the parent insulating cuprates, which is on the order of 0.13 eV (neutron scattering data). Calculation of the spin susceptibility using composite operators is quite a difficult task. It was suggested (see, e.g., [10, 11]) that the most appropriate means of decoupling the equations of motion is offered by the Zwanzig–Mori method. Based on this approach, it has been ascertained that a peak in the neutron scattering intensity is related primarily to the oscillations of localized momenta, which are inherent in a two-dimensional (2D) spin lattice with short-range antiferromagnetic order correlations. This conclusion is qualitatively different from that derived in the RPA scheme.

We have combined the decoupling of the equations of motion in the projection operator representation [12–14] and the RPA scheme to obtain a qualitatively new expression for the spin susceptibility, which takes into account a dual character of the magnetism in HTSCs. For zero occupation numbers, this expression reduces to a formula for the susceptibility of a 2D system of localized spins. For small values of spin correlators, the formula is equivalent to the standard RPA. In application to the problem of neutron scattering in hole-doped HTSCs, our result agrees with the RPA conclusion: a peak in the scattering intensity observed at an energy of about 40 meV is evidence for the existence of collective spin excitations of a new type (spin exciton) in the superconducting state. This result eliminates the problem of interpreting a rather large value of the U parameter in the RPA scheme.

2. EQUATIONS OF MOTION FOR THE CREATION AND ANNIHILATION OPERATORS: QUASI-PARTICLE ENERGY DISPERSION

The model Hamiltonian is as follows:

$$H = \sum_{i,j,\sigma} t_{ij}\psi_i^{pd,\sigma}\psi_j^{\sigma,pd} + \frac{1}{2}\sum_{i,j} J_{ij}\left[\mathbf{S}_i\cdot\mathbf{S}_j - \frac{n_i n_j}{4}\right] + \frac{1}{2}\sum_{i,j} G_{ij}\delta_i\delta_j = H_t + H_J + H_G, \tag{2.1}$$

where, $\psi_i^{pd,\sigma}$ ($\psi_j^{\sigma,pd}$) are the creation (annihilation) operators for composite quasi-particles in the conduction band. In particular, $\psi_i^{pd,\uparrow}$ can be written approximately as

$$\psi_i^{pd,\uparrow} \approx [X_i^{\uparrow,\downarrow}P_i^{\uparrow,0} - X_i^{\uparrow,\uparrow}P_i^{\downarrow,0}]/\sqrt{2},$$

where $X_i^{p,q}$ and $P_i^{p,q}$ are the Hubbard operators for the d-holes on Cu^{2+} and p-holes on O^{1-} sites. Similar expressions for $\psi_i^{pd,\sigma}$ including the singlet state of Cu^{3+} and the neutral state of oxygen are presented elsewhere [8]. There is no need to write these expression here, since (within the framework of a single-band approximation), the conditions of completeness and normalization ensure that the anticommutator relationships of the creation and annihilation operators appear as those for the upper Hubbard zone:

$$\{\psi_i^{pd,\uparrow}, \psi_j^{\uparrow,pd}\} = \frac{1+\delta_i}{2} + s_i^z,$$

where $\delta_i = \psi_i^{pd,pd}$ is the operator of the number of doped holes (per unit cell); superscript pd refers to singlet formations of the holes on copper and oxygen sites. The second term in Hamiltonian (2.1) describes a spin superexchange interaction, while the last term takes into account interactions of the density–density type.

In order to find energy dispersion, we use the equation

$$i\hbar\frac{\partial\psi_k^{\uparrow,pd}}{\partial t} = [\psi_k^{\uparrow,pd}, (H_t + H_J + H_G)] \tag{2.2}$$

and linearize it using the projection technique. The products of operators, which appear as a result of the calculation of commutators in Eq. (2.2), are projected onto a subspace of the creation and annihilation operators. In particular, the operator product $(\psi_j^{pd,pd} + \psi_j^{\uparrow\uparrow})\psi_s^{\uparrow,pd}$ is written in the form of expansion

$$t_{js}(\psi_j^{pd,pd} + \psi_j^{\uparrow\uparrow})\psi_s^{\uparrow,pd} = \sum_n \varepsilon_{jsn}^t\psi_n^{\uparrow,pd} + \sum_n \Delta_{jsn}^t\psi_n^{pd,\downarrow}, \tag{2.3}$$

where the coefficients ε_{jsn}^t and Δ_{jsn}^t are determined from the condition of equality of the averaged anticommutators of the left and right parts of Eq. (2.3) with the creation and annihilation operators. This method of linearization was previously used in [9, 12, 13]. As a result, we obtain the following expressions:

$$\varepsilon_{jns}^t = \frac{t_{ls}}{P}[P^2 + \langle S_s^z S_l^z\rangle]\delta_{ns},$$
$$\Delta_{jns}^t = \frac{t_{js}}{P}\langle\psi_j^{\downarrow,pd}\psi_s^{\uparrow,pd}\rangle\delta_{jn}, \tag{2.4}$$

where $P = (1+\delta)/2$ are the average values of the anticommutator for the operators of creation and annihilation of composite quasi-particles; δ is the average number of carriers per unit cell. The appearance of spin correlators in the hopping integrals is quite clear from a physical standpoint. In the presence of antiferromagnetic correlations in the system of localized spins, the hopping integrals must vanish [9, 15].

The products of operators containing spin or charge density are projected in parts. For the product of operators $\psi_j^{\uparrow,\downarrow}\psi_s^{\downarrow,pd}$, we have

$$t_{js}\psi_j^{\uparrow,\downarrow}\psi_s^{\downarrow,pd} = t_{js}\psi_j^{\uparrow,\downarrow}\psi_s^{\downarrow,pd}(1-F_t) + t_{js}F_t\psi_j^{\uparrow,\downarrow}\psi_s^{\downarrow,pd} = t_{js}(1-F_t)S_j^+\psi_s^{\downarrow,pd} + [\varepsilon_{jsn}^{tr}\psi_n^{\uparrow,pd} + \Delta_{jsn}^{tr}\psi_n^{pd,\downarrow}], \tag{2.5}$$

where F_t is the decoupling parameter that is introduced in order to retain the terms playing an important role in the RPA. In the projection scheme according to [9, 11–13], these terms are ignored. In what follows, we project only a part of operator (2.5)—namely, the product $t_{js}F_t\psi_j^{\uparrow,\downarrow}\psi_s^{\downarrow,pd}$—and take into account the remain-

ing part as is done in the RPA. Accomplishing simple transformations, we eventually obtain

$$\varepsilon^{tr}_{jsn} = t_{js}\frac{F_t}{P}$$
$$\times[\langle\psi_j^{\uparrow,\downarrow}\psi_s^{\downarrow,\uparrow}\rangle\delta_{ns} + \langle\psi_j^{pd,\uparrow}\psi_s^{\downarrow,pd}\rangle\delta_{nj}], \quad (2.6)$$
$$\Delta^{tr}_{jsn} = -t_{js}\frac{F_t}{P}\langle\psi_j^{\uparrow,pd}\psi_s^{\downarrow,pd}\rangle\delta_{nj}.$$

The proposed scheme is in fact a combination of the RPA and the Zwanzig–Mori projection formalism [16, 17], which yielded RPA results for simple metals. From a physical standpoint, it is intended that the decoupling parameter F_t retain the molecular field effects for spins and doped holes. In addition, this parameter has proved important for providing the condition of stability, since not all projection procedures lead to positive values of the imaginary parts of the charge and spin susceptibility. It seems that, in the general case, three parameters can be introduced, which refer to the kinetic energy (F_t), the exchange interaction (F_J), and the Coulomb interaction (F_G).

Combining all terms obtained upon the above linearization procedure, we eventually obtain the following equation:

$$[\psi_k^{\uparrow,pd}, (H_t + H_J + H_G)]$$
$$= \varepsilon_k\psi_k^{\uparrow,pd} + \Delta_k\psi_{-k}^{pd,\downarrow} + \frac{1-F_t}{N}\sum_{\mathbf{q}} t_{k-q}\psi_{k-q}^{\downarrow,pd}S_q^+ \quad (2.7)$$
$$-\frac{F_J}{N}\sum_{\mathbf{q}} J_q\psi_{k-q}^{\downarrow,pd}S_q^+ + \frac{F_G}{N}\sum_{\mathbf{q}} G_q\psi_{k-q}^{\uparrow,pd}\delta_q,$$

where

$$G_q = \sum_i G_{ij}e^{i\mathbf{q}R_{ij}}, \quad J_q = J_1(\cos q_x a + \cos q_y a). \quad (2.8)$$

In the scheme of decoupling described above, the quasi-particle energy and the order parameter of the superconducting transition are expressed as follows:

$$\varepsilon_k = \sum_l t_{jl}\left[\frac{1+\delta}{2} + \frac{2}{1+\delta}(1+2F_t)\langle S_j^z S_l^z\rangle\right]e^{i\mathbf{k}R_{jl}}$$
$$-\sum_l\left(\frac{2G_{jl}(1-F_G)}{1+\delta}\langle\psi_l^{pd,\uparrow}\psi_j^{\uparrow,pd}\rangle\right. \quad (2.9)$$
$$\left.+\frac{J_{jl}(1-F_J)}{1+\delta}\langle\psi_l^{pd,\downarrow}\psi_j^{\downarrow,pd}\rangle\right)e^{i\mathbf{k}R_{jl}},$$

$$\Delta_k = \frac{1}{PN}\sum_{k'}[J(\mathbf{k}-\mathbf{k}')\langle\psi_{k'}^{\uparrow,pd}\psi_{-k'}^{\downarrow,pd}\rangle$$
$$-J(\mathbf{k}-\mathbf{k}')(1-F_J)\langle\psi_{k'}^{\downarrow,pd}\psi_{-k'}^{\uparrow,pd}\rangle$$
$$-F_G G(\mathbf{k}-\mathbf{k}')\langle\psi_{k'}^{\uparrow,pd}\psi_{-k'}^{\downarrow,pd}\rangle] + \frac{1}{PN} \quad (2.10)$$
$$\times\sum_{k'} t_{k'}[\langle\psi_{k'}^{\downarrow,pd}\psi_{-k'}^{\uparrow,pd}\rangle - F_t\langle\psi_{k'}^{\downarrow,pd}\psi_{-k'}^{\uparrow,pd}\rangle],$$

where

$$t_k = \sum_j t_{ij}\exp(i\mathbf{k}R_{ij})$$

are the Fourier transforms of the hopping integrals. Then, the dispersion law for ε_k can be written in the form typical of strong coupling:

$$\varepsilon_k = 2t_{\text{eff}}^{(1)}(\cos k_x a + \cos k_y a)$$
$$+ 4t_{\text{eff}}^{(2)}\cos k_x a\cos(k_y a) \quad (2.11)$$
$$+ 2t_{\text{eff}}^{(3)}(\cos 2k_x a + \cos 2k_y a) + \ldots,$$

where t_{eff} are the effective band parameters, defined as

$$t_{\text{eff}}^{(1)} = t_1\left[P + \frac{1/2+F_t}{1+\delta}K_1\right]$$
$$-\frac{J_1(1-F_J)+2G_1(1-F_G)}{2N}\sum_{\mathbf{k}'} f_{k'}\cos k'_x a,$$
$$t_{\text{eff}}^{(2)} = t_2\left[P + \frac{1/2+F_t}{1+\delta}K_2\right]$$
$$-\frac{J_2(1-F_J)+2G_2(1-F_G)}{2N}\sum_{\mathbf{k}'} f_{k'}\cos k'_x a\cos k'_y a, \quad (2.12)$$
$$t_{\text{eff}}^{(3)} = t_3\left[P + \frac{1/2+F_t}{1+\delta}K_3\right]$$
$$-\frac{J_3(1-F_J)+2G_3(1-F_G)}{2N}\sum_{\mathbf{k}'} f_{k'}\cos 2k'_x a,$$

and $K_n = 4\langle S_0^z S_n^z\rangle$ are the spin–spin correlation functions. The latter functions are self-consistently calculated via the dynamic spin susceptibility with verification of the condition $\langle S_i^+ S_i^-\rangle = (1-\delta)/2$ (the sum rule). The initial values are chosen on the basis of semiempirical considerations.

It should be noted that, in the general case, the presence of density and spin operators in the right-hand part of Eq. (2.7) can change the expression for quasi-particle energy dispersion and lead to pseudogap effects in the density of states at the Fermi level. Here, as the first approximation, we will consider the case where the molecular field effects are insignificant for the dispersion of quasi-particles but still important for the analy-

sis of susceptibility. According to experimental data available on the pseudogap state in HTSCs, there are grounds to believe that this approximation applies to compounds with a doping index close to optimum.

In concluding this section, let us note an interesting feature in behavior of the area of occupied states in the first Brillouin zone. Assuming that the energy of quasiparticle states is independent of the number of holes and writing the equation for the chemical potential as

$$\delta = \frac{1+\delta}{2}\sum_k f(\varepsilon_k - \mu)$$

one can directly arrive at the conclusion (an analog of Lattinger's theorem for simple metals) that the area bounded by the Fermi contour grows as $2\delta/(1+\delta)$ with increasing δ and the zone is half-occupied at $\delta = 1/3$. In the case under consideration, formulas (2.12) contain spin correlators, the absolute values of which decrease with increasing δ. For this reason, the area bounded by the Fermi contour grows faster than the $2\delta/(1+\delta)$ ratio.

3. DYNAMIC SPIN SUSCEPTIBILITY IN THE NORMAL PHASE ($T > T_c$)

The general expression for the dynamic spin susceptibility (derived as described in Appendix A) is as follows:

$$\chi^{+,-}_{\text{total}}(\omega, \mathbf{q}) = \frac{F(\omega, \mathbf{q}) + L_q}{D(\omega, \mathbf{q}) + \Lambda_q^2 - \omega^2}. \tag{3.1}$$

In this formula, the function L_q is defined as

$$\begin{aligned} L_q &= -2J_1K_1(2-c_q) \\ &- \frac{1}{N}\sum_{\mathbf{k}}(n_{k+q}-n_k)(t_{k+q}-t_k), \end{aligned} \tag{3.2}$$

where $c_q = \cos q_x a + \cos q_y a$ and $n_k = \langle \psi_k^{pd,\sigma}\psi_k^{\sigma,pd}\rangle = Pf_k$ are the occupation numbers. The first and second terms in the right-hand part of Eq. (3.2) can be expected to possess opposite signs (for physical reasons, since the electron hopping proceeds with spin conservation), which favors ferromagnetic correlations between local spins.

The function Λ_q^2 in formula (3.1) is defined as

$$\begin{aligned} \Lambda_q^2 &= \Omega_q^2 + \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k) \\ &\times \{[F_J J_q - t_k(1-F_t)]n_k \\ &- [F_J J_q - t_{k+q}(1-F_t)]n_{k+q}\}. \end{aligned} \tag{3.3}$$

For the parameters t and J used in this study, this quantity has the meaning of the squared frequency of local spin excitations and, hence, is always positive. It was pointed out [18, 19] that the frequency of local spin excitations changes upon the appearance of current carriers.

The magnon mode frequency Ω_q in the absence of carriers can be written as [11]

$$\Omega_q^2 = 2J_1^2\alpha|K_1|(2-c_q)(\Delta_{sp}+2+c_q), \tag{3.4}$$

where Δ_{sp} is a dimensionless spin-gap parameter, which characterizes the proximity of the seeding magnon mode to zero at $Q = (\pi, \pi)$ [11], and α is a dimensionless parameter of decoupling according to Kondo and Yamaji [11, 14, 20, 21], which is determined from the sum rule $\langle s_i^+ s_i^-\rangle = (1-\delta)/2$.

The function $D(\omega, \mathbf{q})$ in formula (3.1) is defined as

$$D(\omega, \mathbf{q}) = \frac{\zeta_{t\varepsilon}}{\zeta(\omega, \mathbf{q})}\eta(\omega, \mathbf{q}) - n_{t\varepsilon}(\omega, \mathbf{q}). \tag{3.5}$$

This function has the dimensionality of energy and depends on the band and exchange integral parameters.

Finally, the function $F(\omega, \mathbf{q})$ in formula (3.1) is defined as

$$F(\omega, \mathbf{q}) = \chi(\omega, \mathbf{q})\frac{\zeta_{t\varepsilon}(\omega, \mathbf{q})}{\zeta(\omega, \mathbf{q})} - \chi_{t\varepsilon}(\omega, \mathbf{q}). \tag{3.6}$$

This quantity represents the renormalized susceptibility of free quasi-particles (expressed in the energy units).

The auxiliary functions entering in Eqs. (3.5) and (3.6) are given by the following expressions:

$$\chi(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}\chi_{kq} = \frac{1}{N}\sum_{\mathbf{k}}\frac{n_{k+q}-n_k}{\omega + \varepsilon_k - \varepsilon_{k+q}}, \tag{3.7}$$

$$\begin{aligned} \eta(\omega, \mathbf{q}) &= \frac{1}{N}\sum_{\mathbf{k}}\eta_{kq} = J_q F_J \chi(\omega, \mathbf{q}) \\ &- \frac{1-F_t}{N}\sum_{\mathbf{k}}\frac{t_{k+q}n_{k+q} - n_k t_k}{\omega + \varepsilon_k - \varepsilon_{k+q}}, \end{aligned} \tag{3.8}$$

$$\zeta(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}\zeta_{kq} = \frac{1}{N}\sum_{\mathbf{k}}\frac{1}{\omega + \varepsilon_k - \varepsilon_{k+q}}, \tag{3.9}$$

$$\chi_{t\varepsilon}(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)(\varepsilon_{k+q}-\varepsilon_k)\chi_{kq}, \tag{3.10}$$

$$n_{t\varepsilon}(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)(\varepsilon_{k+q}-\varepsilon_k)\eta_{kq}, \tag{3.11}$$

$$\zeta_{t\varepsilon}(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)(\varepsilon_{k+q}-\varepsilon_k)\zeta_{kq}. \tag{3.12}$$

Formula (3.1) was previously presented (without derivation) in [22]. It should be noted that this formula

can be written in an alternative form. For this purpose, let us consider the following transformation:

$$\chi_{t\varepsilon}(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)(\varepsilon_{k+q}-\varepsilon_k)\chi_{kq}$$

$$= \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)(\varepsilon_{k+q}-\varepsilon_k-\omega)\chi_{kq}$$

$$+\frac{\omega}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)\chi_{kq} \qquad (3.13)$$

$$= -\frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)(n_{k+q}-n_k)$$

$$+\frac{\omega}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)\chi_{kq},$$

where the first term in the right-hand part coincides with one term in (3.2). Upon the substitution of Eq. (3.13) into formula (3.1), these terms cancel each other. Taking into account that

$$\eta_{t\varepsilon}(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)(\varepsilon_{k+q}-\varepsilon_k)\eta_{kq}$$

$$= -\frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)\{[F_J J_q - t_{k+q}(1-F_t)]n_{k+q} \qquad (3.14)$$

$$-[F_J J_q - t_k(1-F_t)n_k]$$

$$+\frac{\omega}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)\eta_{kq},$$

$$\zeta_{t\varepsilon}(\omega, \mathbf{q}) = \omega\zeta_t(\omega, \mathbf{q}), \qquad (3.15)$$

we find two other terms in formula (3.1) that cancel each other. Using these relations, we can rewrite the spin susceptibility as follows:

$$\chi^{+,-}_{\text{total}}(\omega, \mathbf{q}) = \frac{\omega\chi(\omega, \mathbf{q})\zeta_t(\omega, \mathbf{q}) - [\omega\chi_t(\omega, \mathbf{q}) + 2J_1K_1(2-c_q)]\zeta(\omega, \mathbf{q})}{\omega\eta(\omega, \mathbf{q})\zeta_t(\omega, \mathbf{q}) + [\Omega_q^2 - \omega^2 - \omega\eta_t(\omega, \mathbf{q})]\zeta(\omega, \mathbf{q})}, \qquad (3.16)$$

where

$$\zeta_t(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)\zeta_{kq},$$

$$\chi_t(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)\chi_{kq}, \qquad (3.17)$$

$$\eta_t(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)\eta_{kq}.$$

Although Eq. (3.16) appears to have a more complicated form than Eq. (3.1), the functions entering into the alternative expression are substantially simpler, which makes formula (3.16) more appropriate for numerical calculations. It is interesting to note that, under the assumption of $\varepsilon_k = P_{\text{eff}}t_k$ (which is valid in the Hubbard I approximation), the structure of our formula can be transformed (provided that some functions are also redefined) so as to obtain an expression derived in [14]. However, the relation $\varepsilon_k = P_{\text{eff}}t_k$ is not valid in our case. As can be seen from Eq. (2.12), this relation is justified only by neglecting the spin–spin and other correlation functions in the dispersion law.

4. FORMULA FOR THE SPIN SUSCEPTIBILITY AT $T < T_c$

The general structure of formulas (3.1) and (3.16) is retained at $T < T_c$ (detailed derivation is described in Appendix B). Only the form of auxiliary functions in formula (3.16) have to be changed, whereby Eqs. (3.7), (3.8), and (3.9) in the case of $T < T_c$ are generalized as

$$\chi(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}\chi_{kq}$$

$$= \frac{P}{N}\sum_{\mathbf{k}}S_{xx}\frac{f_{k+q}-f_k}{\omega+i\Gamma+E_k-E_{k+q}}$$

$$+\frac{P}{N}\sum_{\mathbf{k}}S_{yy}\frac{f_k-f_{k+q}}{\omega+i\Gamma-E_k+E_{k+q}} \qquad (4.1)$$

$$+\frac{P}{N}\sum_{\mathbf{k}}S^{(-)}_{yx}\frac{f_k+f_{k+q}-1}{\omega+i\Gamma-E_k-E_{k+q}}$$

$$+\frac{P}{N}\sum_{\mathbf{k}}S^{(+)}_{xy}\frac{1-f_k-f_{k+q}}{\omega+i\Gamma+E_k+E_{k+q}},$$

$$\eta(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}\eta_{kq} = J_qF_j\chi(\omega, \mathbf{q}) - \frac{P(1-F_t)}{N}$$

$$\times\left\{\sum_{\mathbf{k}}S_{xx}\frac{t_{k+q}f_{k+q}-t_kf_k}{\omega+i\Gamma+E_k-E_{k+q}}\right.$$

$$+\sum_{\mathbf{k}} S_{yy}\frac{t_{k+q}(1-f_{k+q})-t_k(1-f_k)}{\omega+i\Gamma-E_k+E_{k+q}} \tag{4.2}$$

$$+\sum_{\mathbf{k}} S_{yx}^{(-)}\frac{t_{k+q}f_{k+q}-t_k(1-f_k)}{\omega+i\Gamma-E_k-E_{k+q}}$$

$$+\sum_{\mathbf{k}} S_{xy}^{(+)}\frac{t_{k+q}(1-f_{k+q})-t_kf_k}{\omega+i\Gamma+E_k+E_{k+q}}\Bigg\},$$

$$\zeta(\omega,\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}\zeta_{kq} = \frac{1}{N}\sum_{\mathbf{k}}\frac{S_{xx}}{\omega+i\Gamma+E_k-E_{k+q}}$$

$$+\frac{1}{N}\sum_{\mathbf{k}}\frac{S_{yy}}{\omega+i\Gamma-E_k+E_{k+q}} \tag{4.3}$$

$$+\frac{1}{N}\sum_{\mathbf{k}}\frac{S_{yx}^{(-)}}{\omega+i\Gamma-E_k-E_{k+q}}$$

$$+\frac{1}{N}\sum_{\mathbf{k}}\frac{S_{xy}^{(+)}}{\omega+i\Gamma+E_k+E_{k+q}}.$$

In order to shorten the writing of expressions for the coherence factors, we use the following notation:

$$\begin{aligned} S_{xx} &= x_kx_{k+q}+z_kz_{k+q},\\ S_{yy} &= y_ky_{k+q}+z_kz_{k+q},\\ S_{xy}^{(+)} &= x_ky_{k+q}-z_kz_{k+q},\\ S_{yx}^{(-)} &= y_kx_{k+q}-z_kz_{k+q}, \end{aligned} \tag{4.4}$$

where

$$\begin{aligned} x_k &= u_k^2 = \frac{1}{2}\left[1+\frac{\varepsilon_k-\mu}{E_k}\right],\\ y_k &= v_k^2 = \frac{1}{2}\left[1-\frac{\varepsilon_k-\mu}{E_k}\right], \end{aligned} \tag{4.5}$$

$$z_k = u_kv_k = \frac{\Delta_k}{2E_k}.$$

Note that the generalized functions obey relations (3.17).

5. NUMERICAL CALCULATIONS AND DISCUSSION OF RESULTS

As an application example, we have calculated the imaginary part of the susceptibility as a function of the frequency and wave vector for HTSCs of the $YBa_2Cu_3O_{6+y}$ type. The Fermi contour for such compounds is known from the photoemission data (see exhaustive review [2]). The unit cell contains two layers of CuO_2, and the tunneling of carriers between these layers leads to splitting of the conduction band into the bonding and antibonding subbands. This splitting is sufficiently large, so that we can restrict the analysis to a single-band approximation. With neglect of the pseudogap effects, energy dispersion can be approximately described using the following set of effective parameters: $t_{\text{eff}}^{(1)} = 250$ meV, $t_{\text{eff}}^{(2)} = -50$ meV, $t_{\text{eff}}^{(3)} = 0$ (these values correspond to the experimentally observed Fermi surface). The parameter P was taken equal to 0.67. The Coulomb interaction was evaluated as

$$G(R) = \frac{e^2}{R}\exp(-\sigma_0R),$$

where $\sigma_0 \approx 10^{10}$ m^{-1} is the screening parameter. It has been found that the role of the Coulomb corrections is relatively small; for this reason, we will not consider possible refinements of the Coulomb pseudopotential. The main effects of renormalization of the hopping integrals are related to the parameter P and the spin correlators K_n, the values of which ($K_1 \approx -0.17$, $K_2 \approx 0.04$) were determined from self-consistent calculations with allowance for the sum rule. Eventually, the self-consistent Hamiltonian parameters were as follows $t_1 = 415$ meV, $t_2 = -72$ meV, $t_3 = 0$, $\mu = 160$ meV. The solution of the integral equation (2.10) by analogy with the case (where $F_t = 1$) studied previously [23–25] for $J_1 > G_1$ and an arbitrary F_t yields

$$\Delta_k = \frac{\Delta_0}{2}(\cos k_aa-\cos k_ya). \tag{5.1}$$

Since the form of the pseudopotential for the Coulomb interaction is unknown, the superconducting gap parameter in the susceptibility calculations is set in accordance with the experimental data as $\Delta_0 = 30$ meV [2]. The possible interval of variation of the decoupling parameter F_t is selected proceeding from the condition of stability of the substance, that is, so as to provide that the imaginary parts of the charge susceptibility (a formula for this quantity obtained using the selected method of projection will be reported in a separate publication) and spin susceptibility will be positive for any frequency and wave vector.

Figure 1 shows the imaginary part of the spin susceptibility, which has been numerically calculated using formula (3.16) for the following values of parameters: $J_1 = 115$ meV, $F_t = 0.3$, $F_J = 0.7$, and $\alpha = 1$. The dashed curve shows the results of calculations for $T = 100$ K, which corresponds to the normal phase; the solid curve refers to $T = 10$ K, which corresponds to $T < T_c$. As can be seen, the superconducting phase exhibits a sharp peak in the susceptibility. The main features of both curves in Fig. 1 agree with the experimental data available for $YBa_2Cu_3O_{6+y}$ with $0.7 < y < 1.0$ (see the exhaustive review [1]).

Figure 2 presents the 2D plots of the imaginary part of the spin susceptibility calculated (with the same val-

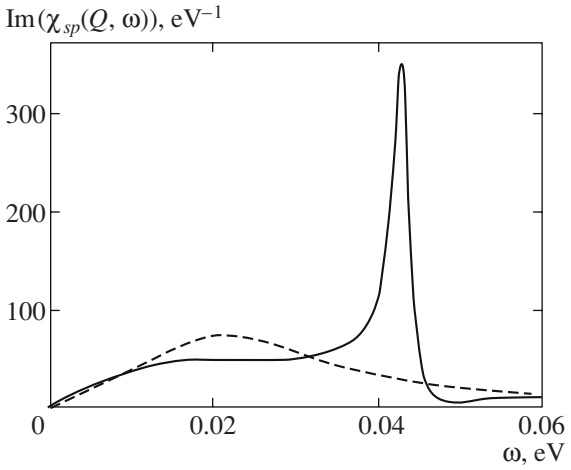

Fig. 1. Imaginary part of the spin susceptibility for the superconducting (T = 10 K, solid curve) and normal (T = 100 K, dashed curve) phases on the wave vector $Q = (\pi, \pi)$.

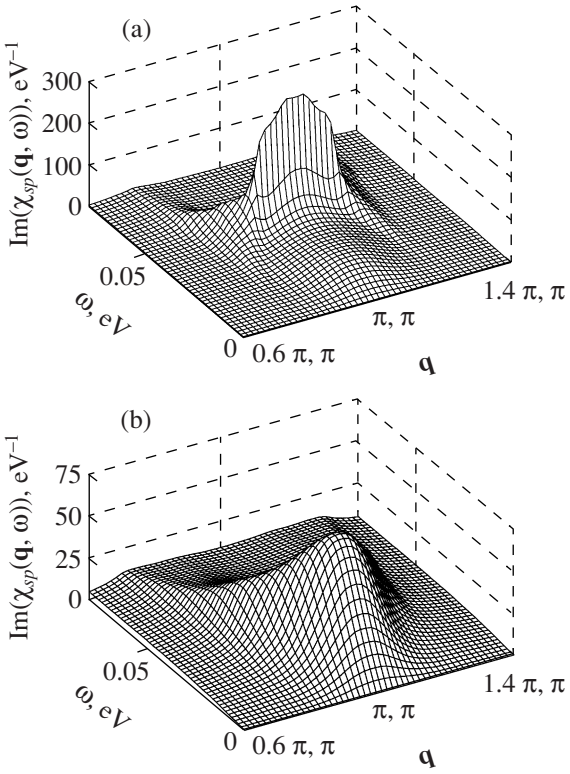

Fig. 2. 2D plots of the imaginary part of the spin susceptibility calculated for the (a) superconducting (T = 10 K) and (b) normal (T = 100 K) phases as functions of the frequency (eV) and wave vector q_x/a (π units) for $q_y/a = \pi$.

ues of parameters) for the normal and superconducting phases. As can be seen, the high-frequency region is characterized by a U-shaped relief, which is more pronounced here than in the RPA. This behavior is related to the Ω_q^2 term in the denominator of formula (3.16), that is, to a manifestation of the correlated excitations of localized spins (short-range order). The U-shaped relief for the normal and superconducting phases is different, which is explained by a change in the $\zeta(\omega, \mathbf{q})$ function that contains the characteristics of charge carriers and, in particular, the superconducting gap parameter. It is interesting that variations in the imaginary part of the spin susceptibility at $T < T_c$ also take place on a scale of energies exceeding the energy gap. This is related to a change in the denominator of formula (3.16), which is common for both localized and itinerant components. A peak observed in the imaginary part of the spin susceptibility for $T < T_c$ explains the origin of resonance in neutron scattering [1]. This peak appears as a result of vanishing of the real part of the denominator of formula (3.16) and, hence, can be interpreted in the same way as in the RPA. In terms of [3], this is manifestation of a spin exciton, since the energy of collective oscillations falls within the superconducting gap ($2\Delta_0 \approx 60$ meV).

It should be emphasized that the pattern of the imaginary part of the spin susceptibility obtained within the framework of our model is richer than that in the RPA scheme. First, the so-called X-shaped envelope of the maximum values of susceptibility (Fig. 3) observed in the neutron scattering [26–28] is more pronounced. The envelope of the maximum values of the susceptibility obtained in our calculations (Fig. 3) fits well the experimental contour observed for $YBa_2Cu_3O_{6.75}$ [26]. Second (which might be especially important for the microscopic theory of Cooper pairing via collective excitations), our calculations (in contrast to the RPA scheme) show that even the normal phase features collective oscillations characteristic of the low-dimensional spin systems (see the divergent U-shaped relief at high frequencies in Fig. 2b). From a physical standpoint, this behavior can be interpreted as a manifestation of the antiferromagnetic correlations in the short-range order. No such short-range order is present in the RPA, where an increase in the imaginary part of the spin susceptibility at low frequencies is conventionally assigned to excitations of the paramagnon type [29]. In our case, the situation is intermediate between paramagnons and short-range AF order correlations. In contrast to the case of short-range order correlations, the real part of the denominator of formula (3.16) does not vanish, but only reaches a minimum as in the case of paramagnons. Our interpretation in favor of the short-range order correlations is based on a similarity in the behavior of envelopes of the maximum susceptibility and Ω_q (see Fig. 3). The energy (frequency) corresponding to the maximum susceptibility in the normal phase can probably be considered as the spin gap (or paramagnon gap) parameter.

To summarize the above considerations, we conclude that the obtained formula for the dynamic spin susceptibility describes a dual character of magnetism in hole-doped HTSCs. On one hand, this is a magnetism of itinerant holes capable of passing to a supercon-

ducting state. On the other hand, there are characteristic features of magnetism inherent in systems consisting of localized moments with short-range antiferromagnetic order correlations. The susceptibility functions have a common denominator and, hence, a common mode of collective spin oscillations. The very strong interplay of local and itinerant spin subsystems makes their separate consideration senseless. The proposed formula reflects a qualitatively new notion of magnetism in hole-doped HTSCs.

ACKNOWLEDGMENTS

The authors are grateful to A.A. Andreev for checking the derivation of formula (3.1) and useful remarks.

This study was supported by the Russian Foundation for Basic Research (project no. 06-02-17197-a) and the Swiss National Science Foundation (grant no. IB7420-110784).

APPENDIX A

Formula of Spin Susceptibility in the Normal Phase ($T > T_c$)

The operator of the spin Fourier component can be written as follows:

$$S_q^+ = \sum_i \psi_i^{\uparrow,\downarrow} e^{-i\mathbf{q}R_i}. \tag{A.1}$$

Calculating the commutator for this operator as

$$[S_q^+, H_t] = \sum_{\mathbf{k}} (t_k - t_{k+q}) \psi_k^{pq,\downarrow} \psi_{k+q}^{\uparrow, pd} \tag{A.2}$$

we obtain the following equation for the Green's function:

$$\begin{aligned}\omega \langle\langle S_q^+ | S_{-q}^- \rangle\rangle &= -\sum_{\mathbf{k}'} (t_{k'+q} - t_{k'}) \langle\langle \psi_{k'}^{pd,\downarrow} \psi_{k'+q}^{\uparrow, pd} | S_{-q}^- \rangle\rangle \\ &+ \sum_{i,l} J_{il} e^{-i\mathbf{q}R_i} \langle\langle S_l^+ S_i^z - S_l^z S_i^+ | S_{-q}^- \rangle\rangle.\end{aligned} \tag{A.3}$$

Assuming that a long-range order is absent, we have

$$\left\langle \sum_i S_i^z \right\rangle = 0. \tag{A.4}$$

First, consider the following Green's function of itinerant electrons:

$$G_{it}(\omega, t) = -\sum_{\mathbf{k}'} (t_{k'+q} - t_{k'}) \langle\langle \psi_{k'}^{pd,\downarrow} \psi_{k'+q}^{\uparrow, pd} | S_{-q}^- \rangle\rangle. \tag{A.5}$$

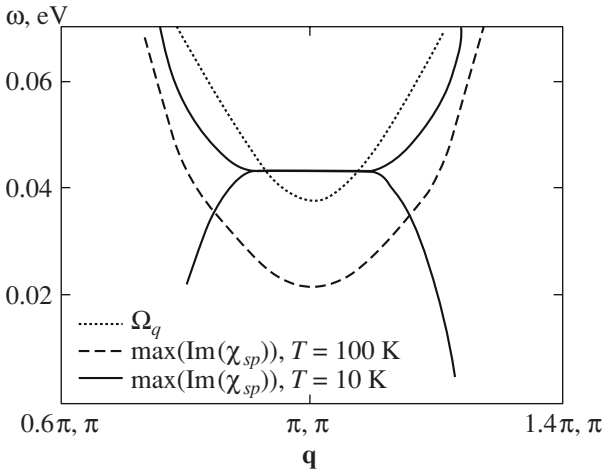

Fig. 3. Envelopes of the maximum values of the imaginary part of susceptibility $\chi_{\text{total}}^{+,-}(\omega, \mathbf{q})$ in the superconducting ($T = 10$ K $< T_c$, solid curve) and normal ($T > T_c = 100$ K, dashed curve) phases in comparison to $\Omega_{\mathbf{q}}$ (dotted curve).

Passing to the lattice-site representation of operators, we obtain

$$\begin{aligned}\psi_k^{pd,\downarrow} \psi_{k+q}^{\uparrow, pd} &= \frac{1}{N} \sum_{ij} \psi_j^{pd,\downarrow} \psi_i^{\uparrow, pd} \\ &\times \exp[i\mathbf{k}R_j - i(\mathbf{k}+\mathbf{q})R_i].\end{aligned} \tag{A.6}$$

As can be readily seen, these operators obey the following identity:

$$\sum_{\mathbf{k}} \psi_{k+q}^{pd,\downarrow} \psi_k^{\uparrow, pd} = 0. \tag{A.7}$$

Below, this identity is used in the following form:

$$\sum_{\mathbf{k}} \langle\langle \psi_k^{pd,\downarrow} \psi_{k+q}^{\uparrow, pd} | S_{-q}^- \rangle\rangle = 0. \tag{A.8}$$

For $T > T_c$, relation (2.7) yields

$$\begin{aligned}&\omega \langle\langle \psi_k^{pd,\downarrow} \psi_{k+q}^{\uparrow, pd} | S_{-q}^- \rangle\rangle \\ &= \frac{i}{2\pi} (\langle \psi_{k+q}^{pd,\uparrow} \psi_{k+q}^{\uparrow, pd} \rangle - \langle \psi_k^{pd,\downarrow} \psi_k^{\downarrow, pd} \rangle) \\ &\times (\varepsilon_{k+q} - \varepsilon_k) \psi_k^{pd,\downarrow} \psi_{k+q}^{\uparrow, pd} \\ &- \frac{1}{N} \{ [F_J J_q - t_k (1 - F_t)] \langle \psi_k^{pd,\downarrow} \psi_k^{\downarrow, pd} \rangle \\ &- [F_J J_q - t_{k+q} (1 - F_t)] \langle \psi_{k+q}^{pd,\uparrow} \psi_{k+q}^{\uparrow, pd} \rangle \} \langle\langle S_q^+ | S_{-q}^- \rangle\rangle \\ &- \frac{1}{N} \sum_{\mathbf{k}'} (\varepsilon_{k'+q} - \varepsilon_{k'}) \langle\langle \psi_{k'}^{pd,\downarrow} \psi_{k'+q}^{\uparrow, pd} | S_{-q}^- \rangle\rangle.\end{aligned} \tag{A.9}$$

The last term in Eq. (A.9) has appeared so as to compensate for the product of operators with $i = j$. Such

products vanish in Eq. (A.6), and this is taken into account in differentiating the products $\psi_k^{pd,\downarrow}\psi_{k+q}^{\uparrow,pd}$ according to the rules established in Section 2. Equations (A.9) are approximate, but we assume that they obey the exact identity (A.8), which yields the following equation:

$$0 = \frac{iN}{2\pi}\chi(\omega,\mathbf{q}) + \frac{1}{N}\eta(\omega,\mathbf{q})\langle\langle S_q^+|S_{-q}^-\rangle\rangle + \zeta(\omega,\mathbf{q})D_{it}(\omega,\mathbf{q}), \quad (A.10)$$

where $D_{it}(\omega,\mathbf{q})$ is an auxiliary Green's function defined as

$$D_{it}(\omega,\mathbf{q}) = -\sum_{\mathbf{k}'}(\varepsilon_{k'+q}-\varepsilon_{k'})\langle\langle\psi_{k'}^{pd,\downarrow}\psi_{k'+q}^{\uparrow,pd}|S_{-q}^-\rangle\rangle$$

(below, this function will also appear in another equation). Using Eq. (A.10), we can rewrite this function as

$$D_{it}(\omega,t) = -\frac{1}{\zeta(\omega,\mathbf{q})} \times\left\{\frac{iN}{2\pi}\chi(\omega,\mathbf{q}) + \frac{1}{N}\eta(\omega,\mathbf{q})\langle\langle S_{\mathbf{q}}^+|S_{-\mathbf{q}}^-\rangle\rangle\right\}. \quad (A.11)$$

For brevity, Eqs. (A.10) and (A.11) are written using the functions $\chi(\omega,\mathbf{q})$, $\eta(\omega,\mathbf{q})$, and $\zeta(\omega,\mathbf{q})$ defined in Eqs. (3.7)–(3.9).

In order to establish new relations, consider the following second derivative with respect to time:

$$-\frac{\partial^2}{\partial^2 t}S_q^+ = \omega^2 S_q^+ = [[S_q^+,H],H]. \quad (A.12)$$

The corresponding equation for the Green's function is as follows:

$$\omega\left\langle\left\langle i\frac{\partial}{\partial t}S_q^+\middle|S_{-q}^-\right\rangle\right\rangle = \omega^2\langle\langle S_{-q}^+|S_{-q}^-\rangle\rangle$$
$$= \omega\langle\langle[S_q^+,H]|S_{-q}^-\rangle\rangle = \frac{i}{2\pi}\langle[[S_q^+,H],S_{-q}^-]\rangle$$
$$-\sum_{\mathbf{k}'}(t_{k'+q}-t_{k'})\langle\langle\psi_{k'}^{pd,\downarrow}\psi_{k'+q}^{\uparrow,pd}|S_{-q}^-\rangle\rangle$$
$$+\sum_{i,l}J_{il}e^{-i\mathbf{q}R_i}\langle\langle[(S_l^+S_i^z - S_l^zS_i^z),H]|S_{-q}^-\rangle\rangle. \quad (A.13)$$

Consider the commutator

$$\langle[[S_q^+,H],S_{-q}^-]\rangle = -2NJ_1K_1(2-c_q)$$
$$+2N\sum_l t_{0l}n_{0l}(e^{iqR_{0l}}-1) = -2NJ_1K_1(2-c_q) \quad (A.14)$$
$$-\sum_{\mathbf{k}}(n_{k+q}-n_k)(t_{k+q}-t_k),$$

where $n_{0l} = \langle\psi_0^{pd,\downarrow}\psi_l^{\uparrow,pd}\rangle$ are the amplitudes of the probability for the composite hole hopping between sites, $c_q = \cos q_x a + \cos q_y a$, and n_k are the occupation numbers. Such a term was also obtained in [18], but the right-hand side of Eq. (A.14) is more convenient for calculations since it is necessary to restrict the number of neighbors in the first line. The Green's function

$$\sum_{i,l}J_{il}e^{-i\mathbf{q}R_i}\langle\langle[(S_l^+S_i^z - S_l^zS_i^+),H],S_{-q}^-\rangle\rangle = \Omega_q^2\langle\langle S_q^+|S_{-q}^-\rangle\rangle \quad (A.15)$$

has been calculated in [11, 14, 18–21]. We use this function in the form of Eq. (3.4) as proposed in [11].

The second term in the right-hand side of Eq. (A.13) can be calculated by analogy with Eq. (A.9) as

$$-\sum_{\mathbf{k}}(t_{k+q}-t_k)\langle\langle[\psi_{k'}^{pd,\downarrow}\psi_{k'+q}^{\uparrow,pd},H]|S_{-q}^-\rangle\rangle$$
$$= -\sum_{\mathbf{k}}(t_{k+q}-t_k)(\varepsilon_{k+q}-\varepsilon_k)\langle\langle\psi_{k'}^{pd,\downarrow}\psi_{k'+q}^{\uparrow,pd}|S_{-q}^-\rangle\rangle$$
$$+\frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k)\{[F_JJ_q - t_k(1-F_t)]n_k - [F_JJ_q - t_{k+q}(1-F_t)]n_{k+q}\}\langle\langle S_q^+|S_{-q}^-\rangle\rangle, \quad (A.16)$$

where we take into account that $\sum_{\mathbf{k}}t_k = 0$, since the energy is measured from the center of the band.

Substituting Eqs. (3.4) ad (A.16) into Eq. (A.13), we obtain

$$\left\{\omega^2 - \Omega_q^2 - \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k) \times\{[F_JJ_q - t_k(1-F_t)]n_k - [F_JJ_q - t_{k+q}(1-F_t)]n_{k+q}\}\right\}\langle\langle S_q^+|S_{-q}^-\rangle\rangle \quad (A.17)$$
$$= -\frac{i}{2\pi}\left\{2NJ_1K_1(2-c_q) + \sum_{\mathbf{k}}(n_{k+q}-n_k)(t_{k+q}-t_k)\right\}$$
$$-\sum_{\mathbf{k}}(t_{k+q}-t_k)(\varepsilon_{k+q}-\varepsilon_k)\langle\langle\psi_k^{pd,\downarrow}\psi_{k+q}^{\uparrow,pd}|S_{-q}^-\rangle\rangle.$$

Rewriting Eq. (A.9) in a more convenient form as

$$\langle\langle \psi_k^{pd,\downarrow} \psi_{k+q}^{\uparrow,pd} | S_{-q}^- \rangle\rangle = \frac{iN}{2\pi}\chi_{kq} + \frac{1}{N}\eta_{kq}\langle\langle S_q^+ | S_{-q}^- \rangle\rangle + \frac{\zeta_{kq}}{N} D_{it}(\omega, t) \tag{A.18}$$

and substituting it into relation (A.17), we obtain

$$\left\{\omega^2 - \Omega_q^2 - \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k) \times \{[F_J J_q - t_k(1-F_t)]n_k - [F_J J_q - t_{k+q}(1-F_t)]n_{k+q}\} + \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\eta_{kq}\right\}\langle\langle S_q^+ | S_{-q}^- \rangle\rangle$$
$$= -\frac{i}{2\pi}\left\{2NJ_1K_1(2-c_q) + \sum_{\mathbf{k}}(n_{k+q} - n_k)(t_{k+q} - t_k) + \sum_{\mathbf{k}}(t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\chi_{kq}\right\} - \frac{D_{it}(\omega, \mathbf{q})}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\zeta_{kq}\,. \tag{A.19}$$

Using this expression jointly with Eq. (A.11), we can exclude the auxiliary function $D_{it}(\omega, \mathbf{q})$ and obtain an equation for the complete Green's function $\langle\langle S_q^+ | S_{-q}^- \rangle\rangle$:

$$\left\{\omega^2 - \Omega_q^2 - \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k) \times \{[F_J J_q - t_k(1-F_t)]n_k - [F_J J_q - t_{k+q}(1-F_t)]n_{k+q}\} + \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\eta_{kq} - \frac{\zeta_{t\varepsilon}(\omega, q)}{\zeta(\omega, q)}\eta(\omega, \mathbf{q})\right\} \times \langle\langle S_q^+ | S_{-q}^- \rangle\rangle = -\frac{i}{2\pi} \times \left\{-N\frac{\chi(\omega, q)}{\zeta(\omega, q)}\zeta_{t\varepsilon}(\omega, \mathbf{q}) + 2NJ_1K_1(2-c_q) + \sum_{\mathbf{k}}(n_{k+q} - n_k)(t_{k+q} - t_k) + N\chi_{t\varepsilon}(\omega, \mathbf{q})\right\}. \tag{A.20}$$

Finally, using the well-known relation between the Green's function $\langle\langle S_q^+ | S_{-q}^- \rangle\rangle$ and the transverse spin susceptibility, we obtain formula (3.1).

APPENDIX B

Formula of Spin Susceptibility in the Superconducting Phase ($T < T_c$)

Considering the superconducting phase, it is convenient to introduce the Bogolyubov quasi-particle operators and use them to express the operator product as

$$\psi_k^{pd,\downarrow}\psi_p^{\uparrow,pd} = u_k u_p \alpha_k^{pd,\downarrow}\alpha_p^{\uparrow,pd} - u_k v_p \alpha_k^{pd,\downarrow}\alpha_{-p}^{pd,\downarrow} + v_k u_p \alpha_{-k}^{\uparrow,pd}\alpha_p^{\uparrow,pd} - v_k v_p \alpha_{-k}^{\uparrow,pd}\alpha_{-p}^{pd,\downarrow} \tag{B.1}$$

and to construct equations for the following Green's functions:

$$\langle\langle \alpha_k^{pd,\downarrow}\alpha_p^{\uparrow,pd} | S_{-q}^- \rangle\rangle, \quad \langle\langle \alpha_k^{pd,\downarrow}\alpha_{-p}^{pd,\downarrow} | S_{-q}^- \rangle\rangle,$$
$$\langle\langle \alpha_{-k}^{\uparrow,pd}\alpha_p^{\uparrow,pd} | S_{-q}^- \rangle\rangle, \quad \langle\langle \alpha_{-k}^{\uparrow,pd}\alpha_{-p}^{pd,\downarrow} | S_{-q}^- \rangle\rangle.$$

It should be borne in mind that the case of like indices ($i = j$) in Eq. (A.6) corresponds to the zero contribution and has to be excluded in taking derivatives. An equation for the Green's function $\langle\langle \alpha_k^{pd,\downarrow}\alpha_p^{\uparrow,pd} | S_{-q}^- \rangle\rangle$ is as follows:

$$(\omega + E_k - E_p)\langle\langle \alpha_k^{pd,\downarrow}\alpha_p^{\uparrow,pd} | S_{-q}^- \rangle\rangle = \frac{i}{2\pi}(u_k u_p + v_k v_p)(n_p - n_k) + \frac{1}{N}(u_k u_p + v_k v_p) \times \{[F_J J_q - t_p(1-F_t)]n_p - [F_J J_q - t_k(1-F_t)]n_k\} \times \langle\langle S_q^+ | S_{-q}^- \rangle\rangle + (u_k u_p + v_k v_p)\frac{1}{N}D_{it}(\omega, \mathbf{q}), \tag{B.2}$$

where $n_k = \langle \alpha_k^{pd,\sigma}\alpha_k^{\sigma,pd} \rangle = Pf_k$ are the occupation numbers in the superconducting state, $E_k = \sqrt{(\varepsilon_k - \mu^2) + |\Delta_k|^2}$, and f_k is the Fermi function defined as

$$f_k = [1 + \exp E_k/k_B T]^{-1}. \tag{B.3}$$

By the same token, equations for the other three Green's function are written as follows:

$$(\omega + E_k + E_{-p})\langle\langle \alpha_k^{pd,\downarrow}\alpha_{-p}^{pd,\downarrow} | S_{-q}^- \rangle\rangle = \frac{i}{2\pi}(u_k v_p - v_k u_p)(n_{-p} + n_k - P) + \frac{1}{N}(u_k v_p - v_k u_p) \times \{[F_J J_q - t_k(1-F_t)]n_k - [F_J J_q - t_p(1-F_t)](P - n_{-p})\} \times \langle\langle S_q^+ | S_{-q}^- \rangle\rangle + (u_k v_p - v_k u_p)\frac{1}{N}D_{it}(\omega, \mathbf{q}), \tag{B.4}$$

$$(\omega - E_{-k} - E_p)\langle\langle \alpha_{-k}^{\uparrow,pd}\alpha_p^{\uparrow,pd} | S_{-q}^- \rangle\rangle = \frac{i}{2\pi}(u_k v_p - v_k u_p)(P - n_{-p} - n_k)$$

$$+\frac{1}{N}(u_k v_p - v_k u_p)\{[F_J J_q - t_k(1-F_t)] \times (P-n_{-k}) - [F_J J_q - t_p(1-F_t)]n_p\}\langle\langle S_q^+|S_{-q}^-\rangle\rangle + (u_k v_p - v_k u_p)\frac{1}{N}D_{it}(\omega,\mathbf{q}),$$

$$(\omega + E_{-k} - E_{-p})\langle\langle \alpha_{-k}^{\uparrow,pd}\alpha_{-p}^{pd,\downarrow}|S_{-q}^-\rangle\rangle = \frac{i}{2\pi}(u_k u_p + v_k v_p)(n_p - n_k) + \frac{1}{N}(u_k u_p + v_k v_p) \times \{[F_J J_q - t_k(1-F_t)](P-n_k) - [F_J J_q - t_p(1-F_t)](P-n_p)\}\langle\langle S_q^+|S_{-q}^-\rangle\rangle + (u_k u_p + v_k v_p)\frac{1}{N}D_{it}(\omega,\mathbf{q}). \quad \text{(B.6)}$$

Multiplying Eqs. (B.2), (B.4), (B.5), and (B.6) by $u_k u_p/(\omega + E_k - E_p)$, $-u_k v_p/(\omega + E_k + E_p)$, $v_k u_p/(\omega - E_k - E_p)$, and $-v_k v_p/(\omega + E_k - E_p)$, respectively, and summing the products, we obtain a generalization of Eq. (A.9) to the case of a superconducting state:

$$\langle\langle \psi_k^{pd,\downarrow}\psi_{k+q}^{\uparrow,pd}|S_{-q}^-\rangle\rangle = \frac{i}{2\pi}\chi_{kq} + \frac{1}{N}\eta_{kq}(\omega,q)\langle\langle S_q^+|S_{-q}^-\rangle\rangle + \frac{\zeta_{kq}(\omega,q)}{N}G_{it}(\omega,\mathbf{q}). \quad \text{(B.7)}$$

Note that the structures of expressions (A.18) and (B.7) are identical. As a result, we obtain the generalized functions (4.1). (4.2), and (4.3).

Instead of Eq. (A.16), we obtain for $T < T_c$ the following relation:

$$-\sum_{\mathbf{k}}(t_{k+q}-t_k)\langle\langle[\psi_{k'}^{pd,\downarrow}\psi_{k'+q}^{\uparrow,pd}], H|S_{-q}^-\rangle\rangle = -\sum_{\mathbf{k}}(t_{k+q}-t_k)\{(E_{k+q}-E_k)u_k u_{k+q} \times \langle\langle \alpha_k^{pd,\downarrow}\alpha_{k+q}^{\uparrow,pd}|S_{-q}^-\rangle\rangle + (E_{k+q}+E_k)u_k v_{k+q} \times \langle\langle \alpha_k^{pd,\downarrow}\alpha_{-k-q}^{pd,\downarrow}|S_{-q}^-\rangle\rangle\} - \sum_{\mathbf{k}}(t_{k+q}-t_k)\{(E_{k+q}+E_k)v_k u_{k+q} \times \langle\langle \alpha_{-k}^{\uparrow,pd}\alpha_{k+q}^{\uparrow,pd}|S_{-q}^-\rangle\rangle + (E_{k+q}-E_k)v_k v_{k+q} \times \langle\langle \alpha_{-k}^{\uparrow,pd}\alpha_{-k-q}^{pd,\downarrow}|S_{-q}^-\rangle\rangle\} + \frac{P}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k) \times \{[F_J J_q - t_k(1-F_t)][f_k(x_k-y_k)+y_k] - [F_J J_q - t_{k+q}(1-F_t)][f_{k+q}(x_{k+q}-y_{k+q})+y_{k+q}]\} \times \langle\langle S_q^+|S_{-q}^-\rangle\rangle, \quad \text{(B.8)}$$

where the Green's functions $\langle\langle \alpha_k^{pd,\downarrow}\alpha_p^{\uparrow,pd}|S_{-q}^-\rangle\rangle$, $\langle\langle \alpha_k^{pd,\downarrow}\alpha_{-p}^{pd,\downarrow}|S_{-q}^-\rangle\rangle$, $\langle\langle \alpha_{-k}^{\uparrow,pd}\alpha_p^{\uparrow,pd}|S_{-q}^-\rangle\rangle$ and $\langle\langle \alpha_{-k}^{\uparrow,pd}\alpha_{-p}^{pd,\downarrow}|S_{-q}^-\rangle\rangle$ are determined from Eqs. (B.2), (B.4), (B.5), and (B.6), respectively. Finally, Eq. (B.8) takes the following form:

$$-\sum_{\mathbf{k}}(t_{k+q}-t_k)\langle\langle[\psi_{k'}^{pd,\downarrow}\psi_{k'+q}^{\uparrow,pd}], H|S_{-q}^-\rangle\rangle = -\sum_{\mathbf{k}}(t_{k+q}-t_k)\left\{\frac{i}{2\pi}\chi_{Ekq} + \frac{1}{N}\eta_{Ekq}\langle\langle S_q^+|S_{-q}^-\rangle\rangle + \zeta_{Ekq}\frac{1}{N}D_{it}(\omega,q)\right\} + \frac{P}{N}\sum_{\mathbf{k}}(t_{k+q}-t_k) \times \left[(J_q - t_k)f_k\frac{\varepsilon_k-\mu}{E_k} - (J_q - t_{k+q})f_{k+q}\frac{\varepsilon_{k+q}-\mu}{E_{k+q}} - t_k y_k + t_{k+q}y_{k+q}\right]\langle\langle S_q^+|S_{-q}^-\rangle\rangle, \quad \text{(B.9)}$$

where

$$\chi_{Ekq} = PS_{xx}(E_{k+q}-E_k)\frac{f_{k+q}-f_k}{\omega + i\Gamma + E_k - E_{k+q}} + PS_{yy}(E_k - E_{k+q})\frac{f_k - f_{k+q}}{\omega + i\Gamma - E_k + E_{k+q}} + PS_{yx}^{(-)}(E_{k+q}+E_k)\frac{f_k + f_{k+q} - 1}{\omega + i\Gamma - E_k - E_{k+q}} - PS_{xy}^{(+)}(E_{k+q}+E_k)\frac{1 - f_k - f_{k+q}}{\omega + i\Gamma + E_k + E_{k+q}}, \quad \text{(B.10)}$$

$$\pi_{Ekq} = PS_{xx}(E_{k+q}-E_k)\frac{t_{k+q}f_{k+q} - t_k f_k}{\omega + i\Gamma + E_k - E_{k+q}} + PS_{yy}(E_k - E_{k+q})\frac{t_{k+q}(1-f_{k+q}) - t_k(1-f_k)}{\omega + i\Gamma - E_k + E_{k+q}} + PS_{yx}^{(-)}(E_{k+q}+E_k)\frac{f_{k+q}f_{k+q} - t_k(1-f_k)}{\omega + i\Gamma - E_k - E_{k+q}} - PS_{xy}^{(+)}(E_{k+q}+E_k)\frac{t_{k+q}(1-f_{k+q}) - t_k f_k}{\omega + i\Gamma + E_k + E_{k+q}}, \quad \text{(B.11)}$$

$$\zeta_{Ekq} = (E_{k+q}-E_k)\frac{S_{xx}}{\omega + i\Gamma + E_k - E_{k+q}}$$

$$+(E_k - E_{k+q})\frac{S_{yy}}{\omega + i\Gamma - E_k - E_{k+q}}$$
$$+(E_k + E_{k+q})\frac{S_{yx}^{(-)}}{\omega + i\Gamma - E_k - E_{k+q}} \quad \text{(B.12)}$$
$$+(-E_k - E_{k+q})\frac{S_{xy}^{(+)}}{\omega + i\Gamma + E_k + E_{k+q}}.$$

Then, we have the following equation analogous to Eq. (A.20):

$$\left\{\omega^2 - \Lambda_q^2 + \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)\eta_{Ekq}\right\}\langle\langle S_q^+ | S_{-q}^-\rangle\rangle$$
$$= -\frac{i}{2\pi}\Bigg\{2NJ_1K_1(2 - c_q)$$
$$+\sum_{\mathbf{k}}(n_{k+q} - n_k)(t_{k+q} - t_k) \quad \text{(B.13)}$$
$$+\sum_{\mathbf{k}}(t_{k+q} - t_k)\chi_{Ekq}\Bigg\} - \frac{D_{it}(\omega, \mathbf{q})}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)\zeta_{Ekq},$$

where Λ_q^2 is determined by the following formula (replacing Eq. (3.3)):

$$\Lambda_q^2 = \Omega_q^2 + \frac{P}{N}\sum_{\mathbf{k}}(t_p - t_k)\Bigg\{(x_k x_p + z_k z_p)$$
$$\times\left[(J_q - t_k)\left(f_k - \frac{1}{2}\right) - (J_q - t_p)\left(f_p - \frac{1}{2}\right)\right]\Bigg\}$$
$$+\frac{P}{N}\sum_{\mathbf{k}}(t_p - t_k)\Bigg\{(x_k y_p - z_k z_p)\left[(J_q - t_k)\left(f_k - \frac{1}{2}\right)\right.$$
$$\left.-(J_q - t_p)\left(\frac{1}{2} - f_p\right)\right]\Bigg\} \quad \text{(B.14)}$$
$$+\frac{P}{N}\sum_{\mathbf{k}}(t_p - t_k)\Bigg\{(y_k x_p - z_k z_p)\left[(J_q - t_k)\left(\frac{1}{2} - f_k\right)\right.$$
$$\left.-(J_q - t_p)\left(f_p - \frac{1}{2}\right)\right]\Bigg\}$$
$$+\frac{P}{N}\sum_{\mathbf{k}}(t_p - t_k)\Bigg\{(y_k y_p + z_k z_p)\left[(J_q - t_k)\left(\frac{1}{2} - f_k\right)\right.$$
$$\left.-(J_q - t_p)\left(\frac{1}{2} - f_p\right)\right]\Bigg\}.$$

Note that, while expression (3.2) for L_q remains unchanged,

$$L_q = -2J_1K_1(2 - c_q)$$
$$-\frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)[n_{k+q} - n_k], \quad \text{(B.15)}$$

the occupation numbers in this formula for $T < T_c$ are calculated, using a different rule, as

$$n_k = \langle\psi_k^{pd,\uparrow}\psi_k^{\uparrow,pd}\rangle$$
$$= P\langle(u_k\alpha_k^{pd,\uparrow} - v_k\alpha_{-k}^{\downarrow,pd})(u_k\alpha_k^{\uparrow,pd} - v_k\alpha_{-k}^{pd,\downarrow})\rangle \quad \text{(B.16)}$$
$$= u_k^2\frac{P}{1 + \exp(E_k/k_BT)} + v_k^2\frac{P}{1 + \exp(-E_k/k_BT)}.$$

The general form of expressions (3.5) and (3.6) is also retained, but the auxiliary functions change to

$$\chi_{tE}(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)\chi_{Ekq}, \quad \text{(B.17)}$$

$$\eta_{tE}(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)\eta_{Ekq}, \quad \text{(B.18)}$$

$$\zeta_{tE}(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)\zeta_{Ekq}, \quad \text{(B.19)}$$

and the functions $\chi_{t\varepsilon}(\omega, \mathbf{q})$, $\eta_{t\varepsilon}(\omega, \mathbf{q})$, and $\zeta_{t\varepsilon}(\omega, \mathbf{q})$ have to be replaced by $\chi_{tE}(\omega, \mathbf{q})$, $\eta_{tE}(\omega, \mathbf{q})$, and $\zeta_{tE}(\omega, \mathbf{q})$, respectively. Thus, the formulas for the susceptibility in both phases are similar and the auxiliary functions $D(\omega, \mathbf{q})$ and $F(\omega, \mathbf{q})$ are given by the following expressions:

$$D(\omega, \mathbf{q}) = \frac{\zeta_{tE}(\omega, \mathbf{q})}{\zeta(\omega, \mathbf{q})}\eta(\omega, \mathbf{q}) - \eta_{tE}(\omega, \mathbf{q}), \quad \text{(B.20)}$$

$$F(\omega, \mathbf{q}) = \chi(\omega, \mathbf{q})\frac{\zeta_{tE}(\omega, \mathbf{q})}{\zeta(\omega, \mathbf{q})} - \chi_{tE}(\omega, \mathbf{q}). \quad \text{(B.21)}$$

Upon simplifications, the formula eventually acquires the same form as that for the normal phase (see Eq. (3.16)).

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Translated by P. Pozdeev